

=> S 11 and 13
405111 L1
13647 L3
L4
31 L1 AND L3
=> S 14 and (racemi? or resol?)
39318 RACEMI?
442012 RESOL?
L5
23 L4 AND (RACEMI? OR RESOL?)

=> d 1-23 libb abs hitstr

L5 ANSWER 1 OF 23 CAPUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003-417577 CAPUS
DOCUMENT NUMBER: 139-6672
TITLE: Process for the Synthesis of (R)-1-(3,5-bis(trifluoromethyl)phenyl)ethan-1-ol and esters thereof by dynamic kinetic resolution
INVENTOR(S): Karel Maria Broxterman, Quirinus Bernardus, Verzijl, Gerardus
PATENT ASSIGNEE(S): MERCK & CO., Inc., USA
PCT Int. Appl., 44 pp.
CODEN: PIXDD2
Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. 2003043575
WO 2003043575

A2 20031016

WO 2002-US36969

20021115

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TU, TM, TN, TR, TT, TZ, UA, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TU, TM
RW: GH, KE, LS, MW, MZ, SD, SI, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CI, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SB, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-333039P P 20011119

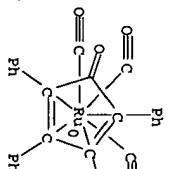
OTHER SOURCE(S): CASREACT 139-6672; MARPAT 139-6672
AB (R)-1-(3,5-Bis(trifluoromethyl)phenyl)ethan-1-ol and esters thereof were obtained via dynamic kinetic **resoln.** These compds. are useful as intermediate in the synthesis of compds. which possess pharmacological activity. Thus, 1,3-(P3C)2C6H4 was brominated and the resulting 3,5-(P3C)3C6H2Br subjected to Grignard reaction with Ac2O to give 3,5-(P3C)3C6H2COAc or with MeCtO to give 3,5-(P3C)3C6H2CHMeOH. 3,5-(P3C)3C6H2COAc was subjected to transfer hydrogenation in presence of [RuCl2(PPh3)2] and (R,S)-HANChMeCOAc to give (R,S)-3,5-(P3C)3C6H2CHMeOH which was subjected to kinetic **resoln.** with CH2Cl2/CHMeOAc in presence of Novozym35 to give (R)-3,5-(P3C)3C6H2CHMeOAc with 99% ee.

IT 9001-63-1 Novozym35 12321-08-3 37362-03-1
37366-09-9, Benzenetrichromium dichloride dimer 37375-79-4
52462-29-0, P-Cymenetrichromium dichloride dimer 52462-30-3
52462-31-4 67421-02-7 88946-78-5
88946-79-6 88946-80-9 10449-77-2
12265-36-1
RL: CAT (catalyst use); USGS (uses)
(process for the synthesis of (R)-1-(3,5-bis(trifluoromethyl)phenyl)eth

RN 9001-62-1 CAPUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

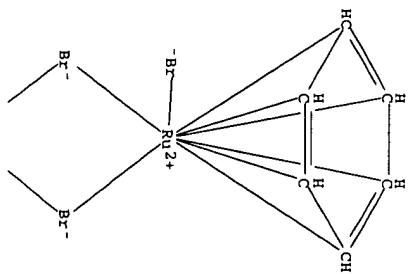
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 12321-08-3 CAPUS
CN Ruthenium, tricarbonyl[(2,3,4,5-eta.)-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-one]- (9CI) (CA INDEX NAME)

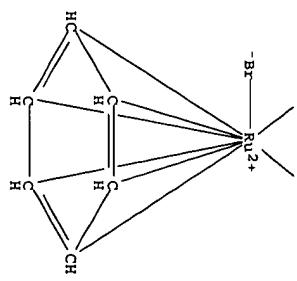


RN 37362-03-1 CAPUS
CN Ruthenium, bis(eta-6-benzene)di-mu-bromodibromido- (9CI) (CA INDEX NAME)

PAGE 1-A

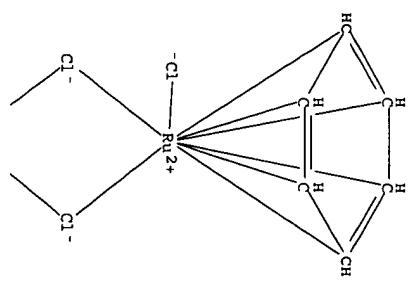


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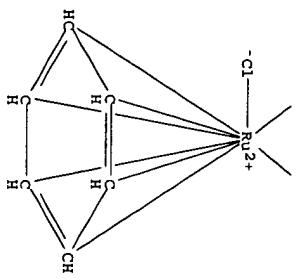


RN 37366-09-9 CAPLUS
CN Ruthenium, bis(eta-6-benzene)di-mu-chlorodichloro- (9CI) (CA INDEX NAME)

PAGE 1-A

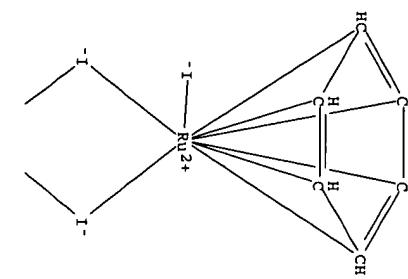


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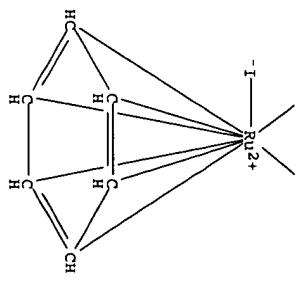


RN 37375-79-4 CAPLUS
CN Ruthenium, bis(eta-6-benzene)di-mu-iododiodo- (9CI) (CA INDEX NAME)

PAGE 1-A

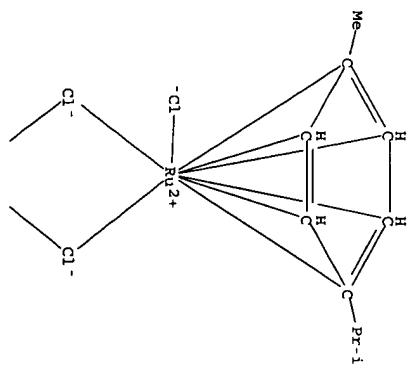


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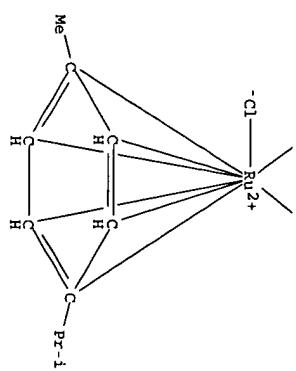


RN 52462-29-0 CAPPUJS
CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene]di-. (9CI) (CA INDEX NAME)

PAGE 1-A

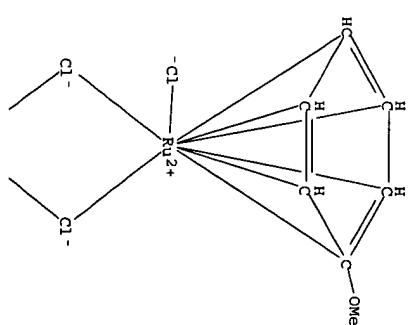


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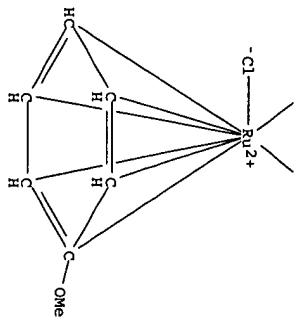


RN 52462-30-3 CAPPUJS
CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-methoxybenzene]di-. (9CI) (CA INDEX NAME)

PAGE 1-A



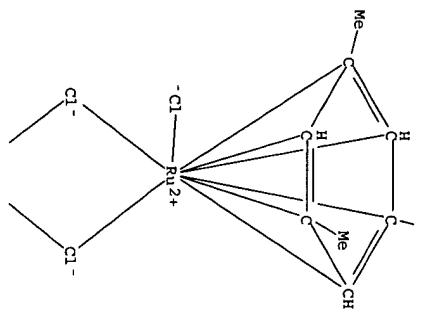
PAGE 2-A



RN 52462-31-4 CAPLUS
CN Ruthenium, di-*mu*-chlorodichlorobis[(1,2,3,4,5,6-*eta*.)-1,3,5-trimethylbenzene]di- (9CI) (CA INDEX NAME)

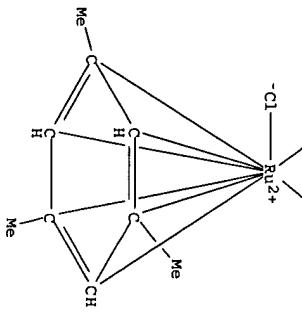
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PAGE 2-A



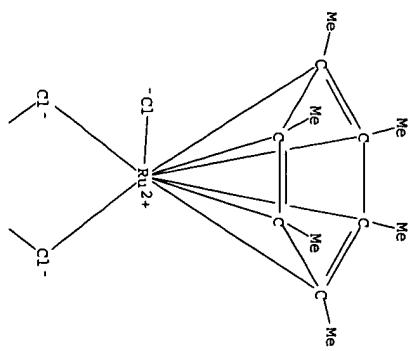
PAGE 3-A

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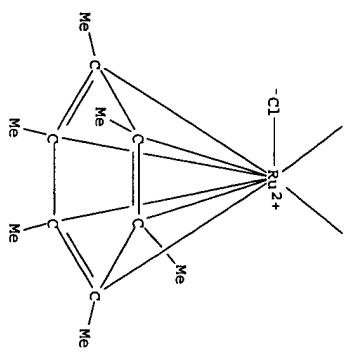
RN 67421-02-7 CAPLUS
CN Ruthenium, di-*mu*-chlorodichlorobis[(1,2,3,4,5,6-*eta*.)-hexamethylbenzene]di- (9CI) (CA INDEX NAME)

PAGE 1-A



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PAGE 2-A

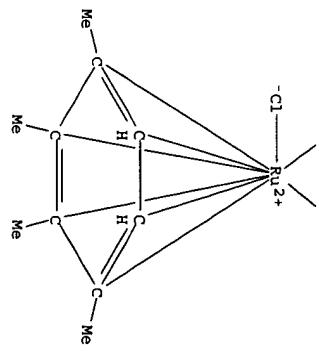


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RN
88946-78-5 CAPRUS
CN
Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1,2,3,4-
tetramethylbenzenedi- (9CI) (CA INDEX NAME)]

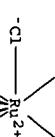
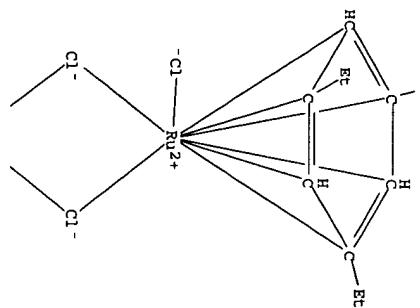
PAGE 3-A



RN 88946-79-6 CAPIUS
CN Ruthenium di-mu-chlorodichlorobis((1,2,3,4,5,6-eta.)-1,3,5-triethylbenzenedi-(9CI) (CA INDEX NAME)

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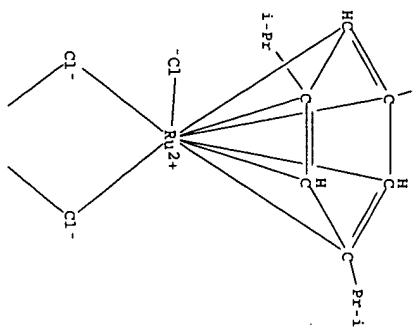


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RN 88946-80-9 CAPIUS
CN Ruthenium di-mu-chlorodichlorobis((1,2,3,4,5,6-eta.)-1,3,5-tris(1-methylethyl)benzenedi-(9CI) (CA INDEX NAME)

Et

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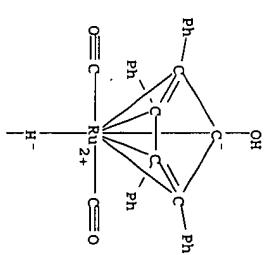
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PAGE 1-A

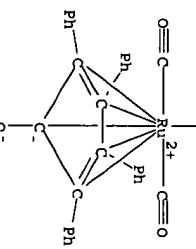


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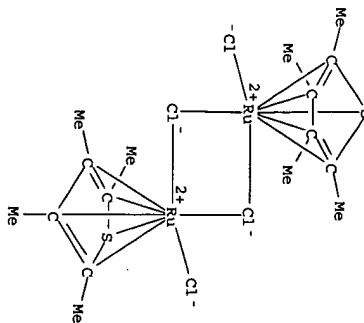
RN 104439-77-2 C4PLUS
CN Ruthenium, tetracarbonyl, mu-hydro[[(1,2,3,4,5-eta)-1-hydroxylato-
2,3',4,5-tetraphenyl-1-2,4-cyclopentadien-1-yl][[(1,2,3,4,5-eta)-1-hydroxy-
2,3',4,5-tetraphenyl-1-2,4-cyclopentadien-1-yl]di-(gCl)] (CA INDEX NAME)



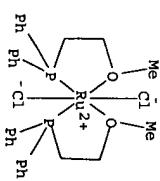
PAGE 1-A



CN Ruthenium, di-*mu*-chlorodichlorobis[(2,3,4,5-*eta*)-tetramethylthiophene-*eta*.*eta*.*eta*.*eta*]-, stereoisomer (9CI) (CA INDEX NAME)



AUTHOR(S): LINDNER, EKKEHARD; GHALEM, ASH
 CORPORATE SOURCE: INSTITUTE OF INORGANIC CHEMISTRY, TUBINGEN, TUBINGEN, GERMANY
 SOURCE: TETRAHEDRON: ASymmetry (2003) CODEN: TASYE3; ISSN: 0957-4166
 PUBLISHER: ELSEVIER SCIENCE LTD.
 DOCUMENT TYPE: Journal Article
 LANGUAGE: English
 ABSTRACT: The RuCl₂(η -1-PH₂CH₂CHOCH₃)₂(diamine) complex forms high yields from the reaction of equimolar amounts of PH₂CH₂CHOCH₃₂ with various kinds of chelating five-membered chelates with ruthenium. These novel



different types of cocatalysts. Whereas complexes with achiral diamines afforded the **racemic** alcs., complexes with chiral diamines (R,R or S,S) allowed the formation of the corresponding enantiomerically enriched secondary alc. (S or R) with ee values of 45%. In order to obtain the secondary alc. with ee of >99%, the kinetic **reson**. of enantiomerically enriched I was performed in a consecutive approach using either the Liase-catalyzed enantioselective transesterification of the alc. with isopropanol acetate as the acyl donor in toluene or the enantioselective hydrolysis of the corresponding acetate in buffer. The de- of the enantiomeric excess (ee) of the resulting enantiomerically enriched secondary alcs. was performed by gas chromatog. using heptakis(2,3-di-O-methyl-6-O-*p*-tert-butyldimethylsilyl)-beta.-cyclodextrin as the chiral stationary phase.

RU: CAY (catalytic use); USES (uses)
 (asim. hydrogenation of an alpha,-beta.-unsatd. ketone by
 diamine (ether-phosphine) ruthenium(II) complexes and lipase-catalyzed
 kinetic reson.)
 RN 9001-62-1 CAPRIUS
 CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT
199011-62-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. hydrogenation of an alpha beta-unsat.)

RN
diamine(ether-phosphine)ruthenium(II) complexes and lipase-catalyzed
kinetic reason.)
10911-62-3 CAPUS
Ruthenium, dichlorobis(12-(methoxy- κ 0)ethyl)diphenylphosphine-
CN

.KAPPA.EPJ-; (05-6-13)- (9C1) (A INDEX NAME

REFERENCE COUNT: 30 THEREFORE

RECORD. ALL CITATIONS AWAY

L5 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:120380 CAPLUS

DOCUMENT NUMBER: 138:283203
TITLE: On the Mechanism of the Unexpected Facile Formation of

meso-Diacetate Products in Enzymatic Acetylation of Alkanediols

AUTHOR(S): Edin, Michaela; Baeckvall, Jan-E.
CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory

SOURCE: Stockholm University, Stockholm, SE-106 91, Swed. *Journal of Organic Chemistry* (2003). 68(6): 2316-2323

PUBLISHER: American Chemical Society
CODEN: JOCEAH ISSN: 0021-9588

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CARRÉCT 138-283203
AB THE MECHANISM OF THE UNEXPECTED FACILE FORMATION OF MESO-DIACETATE PREVIOUSLY OBSR. IN THE ENZYMIC RESON. OF D,L/MESO MIXTS. OF

2,4-pentanediol and 2,5-hexanediol with *Candida antarctica* lipase B has been elucidated. It was found that the formation of meso-diacetate proceeds via different mechanisms for the two diols. Enzyme-catalyzed acylation of AcOO^{d3} labeled (R)-monooacetates of meso-2,4-pentanediol and meso-2,5-hexanediol and anal. of the meso-diacetates obtained show that the former reaction proceeds via intramol. acyl migration while the latter occurs via direct S-acylation of the alc. For the (R)-monooacetate of (R,S)-2,4-pentanediol the intramol. acyl migration was fast and therefore direct S-acylation by the external acyl donor is suppressed. For the hexanediol monooacetate the rate ratio (pseudo E value) between (5R,2R)- and (5R,2S)-S-acetoxyl-2-hexanol was expl. dets. to be $K_R/K_S = 25$, which is about 10-20 times lower than the E value for 2-pentanol and 2-octanol. In a preliminary expt. it was demonstrated that facile acyl migration in the 1,3-diol deriv. can be utilized to prep.

via a chemoenzymic dynamic kinetic asym. transformation of a meso/DL mixt.

IT 104433-77-2

RL: (Reactant); RACT (Reactant or reagent)

(Candida antarctica lipase can form anti-Kazlauskas acetylation

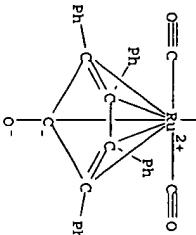
products of 2,4-pentanediol and 2,5-hexanediol)

RN 104433-77-2 CAPLUS

Ruthenium tetracarbonyl-mu-hydro[[1,2,3,4,5-eta]-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-(9CI) (CA INDEX NAME)

CN 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-(9CI) (CA INDEX NAME)

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IT 9001-62-1

RU: CAT (Catalyst use); USES (Uses) (Lipase B; Candida antarctica lipase can form anti-Kazlauskas acetylation products of 2,4-pentanediol and 2,5-hexanediol)

RN 9001-62-1 CAPLUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Ruthenium tetracarbonyl-mu-hydro[[1,2,3,4,5-eta]-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-(9CI) (CA INDEX NAME)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2004 ACS ON STN

ACCESSION NUMBER: 2003-76732 CAPLUS

DOCUMENT NUMBER: 138:137021

TITLE: Process for the reacetalization of secondary alcohols using ruthenium compounds and chelating agents

Kiermeier, Thomas; Gross, Peter; Hoff, Manfred; Monsse, Axel; Dingerdissen, Uwe

DEGUSSA AG, Germany; Degussa AG, Germany; PCT INT. APPL., 22 PP.

CODEN: PIXDZ

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138:137021

Process for the reacetalization of secondary

alcohols using ruthenium compounds and chelating

agents

Kiermeier, Thomas; Gross, Peter; Hoff, Manfred; Monsse, Axel; Dingerdissen, Uwe

DEGUSSA AG, Germany; Degussa AG, Germany; PCT INT. APPL., 22 PP.

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138:137021

Process for the reacetalization of secondary

alcohols using ruthenium compounds and chelating

agents

Kiermeier, Thomas; Gross, Peter; Hoff, Manfred; Monsse, Axel; Dingerdissen, Uwe

DEGUSSA AG, Germany; Degussa AG, Germany; PCT INT. APPL., 22 PP.

CODEN: PIXDZ

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RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

138:137021

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Kiermeier, Thomas; Gross, Peter; Hoff, Manfred; Monsse, Axel; Dingerdissen, Uwe

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CODEN: PIXDZ

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DEGUSSA AG, Germany; Degussa AG, Germany; PCT INT. APPL., 22 PP.

CODEN: PIXDZ

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RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

138:137021

Process for the reacetalization of secondary

alcohols using ruthenium compounds and chelating

agents

Kiermeier, Thomas; Gross, Peter; Hoff, Manfred; Monsse, Axel; Dingerdissen, Uwe

DEGUSSA AG, Germany; Degussa AG, Germany; PCT INT. APPL., 22 PP.

CODEN: PIXDZ

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RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

138:137021

80. degree. in a Schlenk tube for 5 h to give a product having 1% enantiomeric excess. The process was also carried out simultaneously with a kinetic enzymic resolin.

IT 9001-63-1 Chirazyme L-2

RU: CAT (catalyst use); USSS (Uses)

(dynamic kinetic resolin. of secondary alcs. using ruthenium

compds. and chelating agents)

RN 9001-62-1 CAPIUS

lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 37366-09-9 Benzeneruthenium(II) chloride dimer 52462-29-0

13454-84-8

RU: CAT (catalyst use); USSS (Uses)

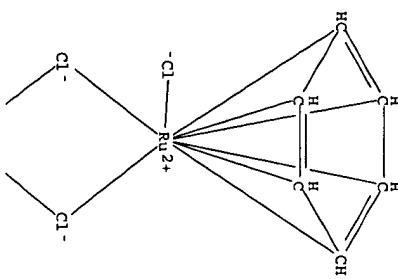
(process for the racemization of secondary alcs. using

ruthenium compds. and chelating agents)

RN 37365-09-9 CAPIUS

Ruthenium, bis(.-eta.6-benzene)di-.mu.-chlorodichlorodi-

(9CI) (CA INDEX NAME)



PAGE 1-A

RN

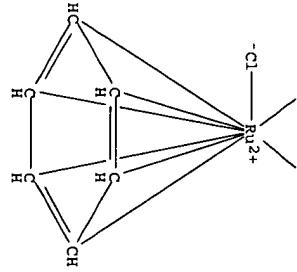
52462-29-0

CAPIUS Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-

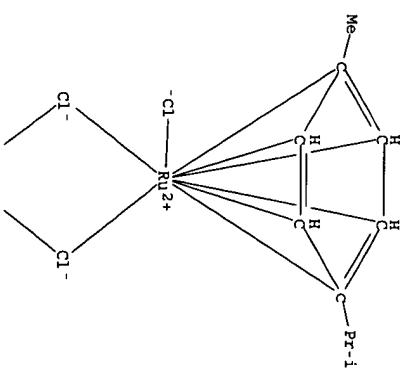
CN

methyl-ethyl)-benzene]di-

(9CI) (CA INDEX NAME)



PAGE 1-A



PAGE 2-A



IT 9001-62-1, Lipase
 RU: CAT (catalyst use); USES (uses)
 (pseudomonas sp.; chemoenzymic dynamic kinetic **resolin**. of
 .beta.-halo alcs. and subsequent conversion of intermediate acetates to
 chiral epoxides)

RN 9001-62-1 CAPLUS
 CN lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 104439-77-2

RU: CAT (catalyst use); USES (uses)
 (racemization catalyst; chemoenzymic dynamic kinetic
resolin. of .beta.-halo alcs. and subsequent conversion of

intermediate acetates to chiral epoxides)

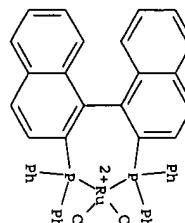
RN 104439-77-2 CAPLUS

Ruthenium, tetracarbonyl-.mu.-hydro((1,2,3,4,5-.eta.)-1-hydroxylato-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl)(1,2,3,4,5-.eta.-1-hydroxy-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl)di-. (9CI) (CA INDEX NAME)



RN 134524-84-8 CAPLUS

Ruthenium, [(1,1'-binaphthalene)-2,2'-diylbis(diphenylphosphine-
 .kappa.P)] dichloro, [SP-4-2-(S)]-(9CI) (CA INDEX NAME)



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE IN THE RE FORMAT
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:880431 CAPLUS

DOCUMENT NUMBER: 138106546

TITLE: Chemoenzymatic Dynamic Kinetic Resolution of

Epoxides
 .beta.-Halo Alcohols. An Efficient Route to Chiral

Pamies, Oscar; Baekvall, Jan-E.

Department of Organic Chemistry, Arrhenius Laboratory,
 Stockholm University, Stockholm, SE-10691, Swed.

Journal of Organic Chemistry (2002), 67(25), 9006-9010

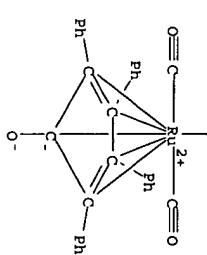
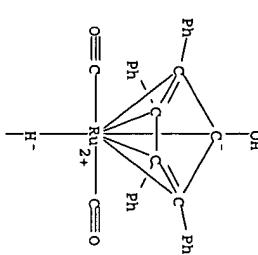
CODEN: JOCEAH, ISSN: 0022-3263

PUBLISHER: American Chemical Society

LANGUAGE: English

OTHER SOURCE (S): CASREACT 138-10546
 AB Enzymic **resolin**. of .beta.-chloro alcs. in combination with

ruthenium-catalyzed alc. isomerization led to a successful dynamic kinetic
resolin. (conversion up to 99% and ee up to 97%). The efficiency
 of the DKR is dramatically reduced when .beta.-bromo alcs. are used. The
 presence of the bromo substituent causes decom. of the ruthenium
 catalysts, which triggers the progressive deactivation of the enzyme. The
 synthetic utility of this procedure has been illustrated by the practical
 synthesis of different chiral epoxides.



REFERENCE COUNT:

43

THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 1-A

L5 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:888574 CAPLUS
DOCUMENT NUMBER: 138:277003
TITLE: Efficient lipase-catalyzed kinetic resolution and dynamic kinetic resolution of .beta.-hydroxy nitriles. Correction of absolute configuration and transformation to chiral .beta.-hydroxy acids and .gamma.-amino alcohols

AUTHOR(S): Pamies, Oscar; Backvall, Jan-E
CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, 106 91, Swed.
Advanced Synthesis & Catalysis (2002), 34(3), 947-952
SOURCE: CODEN: ACSRF7; ISSN: 1615-4150
Wiley-VCH Verlag GmbH & Co. KGaA
Journal

PUBLISHER:

DOCUMENT TYPE: CASPACT 138:271003
LANGUAGE: English

AB Chemoenzymic dynamic kinetic resolution of .beta.-hydroxy nitriles has been carried out using *Candida antarctica* lipase B and a ruthenium catalyst. The use of a hydrogen source to depress ketone formation in the dynamic kinetic resolution yields the acetates in good yield and high enantioselectivity. It is shown that the ruthenium catalyst and the enzyme can be recycled when used in sep. reactions. Enantiomerically pure .beta.-, hydroxy acid derivs. and .gamma.-amino alcs. were prep. from the hydroxy nitriles and acetates. The latter compds. were also used to establish the correct abs. configuration of the hydroxy nitriles and acetates.

IT

RL: CAT (catalyst; use); USGS

(Lipase B; Lipase-catalyzed kinetic resoln. and dynamic

kinetic resoln. of .beta.-hydroxy nitriles and conversion to

chiral .beta.-hydroxy acids and .gamma.-amino alcs.)

RN 9001-62-1 CAPLUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 10439-77-2

RL: CAT (catalyst; use); USGS

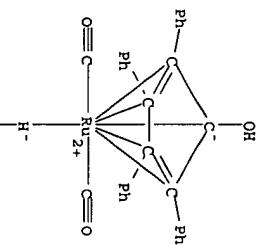
(Lipase-catalyzed kinetic resoln. and dynamic kinetic

resoln. of .beta.-hydroxy nitriles and conversion to chiral

RN 10439-77-2 CAPLUS

CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.]-1-hydroxyato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-(9CI) (CA INDEX NAME)

PAGE 2-A



PAGE 2-A

L5 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:456611 CAPLUS
DOCUMENT NUMBER: 137:884594
TITLE: An efficient and mild ruthenium-catalyzed racemization of amines: application to the synthesis of enantiomerically pure amines

AUTHOR(S): Pamies, Nina; Backvall, Jan-E; Hermanns, Joseph S. M.; Arrhenius Laboratory, Department of Organic Chemistry, Stockholm University, Stockholm, SE-10651, Swed.
Tetrahedron Letters (2002), 43(26), 4699-4702
SOURCE: CODEN: TLELEY; ISSN 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An efficient and mild Ru-catalyzed racemization of amines under

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:456611 CAPLUS
DOCUMENT NUMBER: 137:884594
TITLE: An efficient and mild ruthenium-catalyzed

racemization of amines: application to the synthesis of enantiomerically pure amines

AUTHOR(S): Pamies, Oscar; Bili, Alida H.; Samec, Joseph S. M.; Arrhenius Laboratory, Department of Organic Chemistry, Stockholm University, Stockholm, SE-10651, Swed.
Tetrahedron Letters (2002), 43(26), 4699-4702
SOURCE: CODEN: TLELEY; ISSN 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

transfer hydrogenation conditions is reported. A significant advantage of this new procedure is that the ruthenium hydrogen transfer catalysts allow high functional group tolerance. Interestingly, both primary and secondary amines were efficiently **racemized** under these conditions. We also report on the combination of this new amine racemization with an enzymic kinetic **resoln.** of primary amines.

IT 9001-62-1 Lipase 104419-77-2

RU: Cat. (catalyst, use); USES (Uses)

(ruthenium-catalyzed **racemization** of amines and subsequent **lipase-catalyzed kinetic resoln.**)

RN 9001-62-1 CAPUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

PAGE 1-A

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

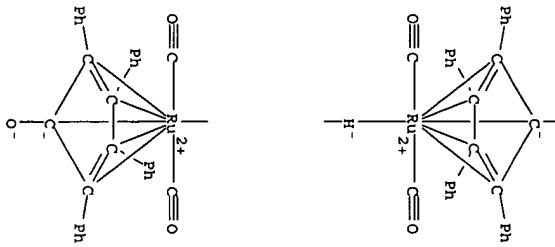
Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

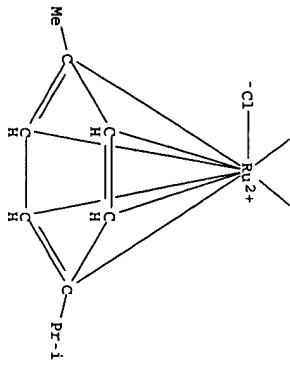
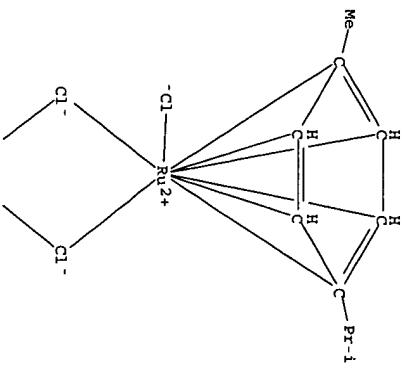
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPUS

Ruthenium, tetracarbonyl-.mu.-hydro[1,(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 34 RECORD: THERE ARE 34 CITED REFERENCES AVAILABLE IN THE RE FORMAT
L5 ANSWER 8 OF 23 CAPUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:03138 CAPUS
DOCUMENT NUMBER: 137:369562
TITLE: Efficient ruthenium-catalyzed **racemization** of secondary alcohols: application to dynamic kinetic resolution
AUTHOR(S): Dijkman, Arne; Elzinga, Jeffrey M.; Li, Yu-Xin; Arends, Isabel W. C. E.; Sheldon, Roger A.
CORPORATE SOURCE: Department of Biotechnology, Biocatalysis and Organic Chemistry, Delft University of Technology, Delft, 2628 Bl, Neth.
SOURCE: Tetrahedron: Asymmetry (2002), 13(8), 879-884
PUBLISHER: ELSEVIER; ISSN: 0957-4186
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three new ruthenium-based catalytic systems are described which are capable of catalyzing the **racemization** of chiral secondary alcohols. In addition, one of these systems, [Tb[NH2(CH2)2RuCl(p-cymene)]/TEMPO, was able to catalyze the *in situ* **racemization** during enzymic **resoln.**, i.e. dynamic kinetic **resoln.**
IT 9001-62-1 Novozym 435
RU: NNU (Other use, unclassified); USES (Uses)
(additive: effect of additives on **racemization** of secondary alics. in presence of ruthenium compds./TEMPO catalytic systems)
IT 52462-29-0
(RU: RCT (Reactant); RACT (Reactant or reagent)
Efficient ruthenium compds./TEMPO catalytic systems for **racemization** of secondary alics. and potential applications to dynamic kinetic **resoln.**)
IT 52462-29-0 CAPUS
Ruthenium, di-mu-chlorodichlorobis[(1,2,3,4,5-.eta.)-1-methyl-4-(1-methyl-ethyl)benzene]di- (9CI) (CA INDEX NAME)



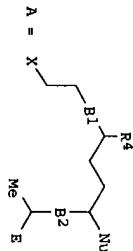


PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002032844	A2	20020425	WO 2001-EP11992	20011016
WO 2002032844	C1	20030821		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DB, DK, DM, DZ, EC, ES, FI, GB, GO, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MK, MZ, NO, NZ, PH, PT, RO, RU, SD, SB, SG, SI, SK, SL, TU, TM, TR, TT, TZ, UA, UG, US, UZ, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MM, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, DE 10051136 A1 20020418 DE 2000-10051136 20001016				
DE 10134172 A1 2001123	DE 2001-10134172 20010713			
AU 200221693 AS 20020429 AU 2002-21693 20031016				
EP 1558144 A1 20031105 EP 2001-987736 20011016				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, DE 2000-10051136 A 20001016 DE 2001-10134172 A 20030713				
WO 2001-EP11992 W 20011016				

PRIORITY APPN. INFO.: DE 2001-10134172 A 20030713

OTHER SOURCE(S): CASREACT 136:34054; MARPAT 136:340534

GT



AB The invention relates to **racemic** and **esp.** **non-racemic**

acyloins, $\text{R}1(\text{O})\text{CR}2\text{OR}1$; $\text{R}1 = \text{H, aryl}$ (esp. Me, Et, Pr), aryl , alkyl , alkyl-aryl , $\text{CH}_2\text{-aryl}$, vinyl , alkynyl , propynyl , allyl , 3,3-dialkylallyl , $\text{C}_3\text{-7-cycloalkyl}$, $\text{CHar}_3\text{-n}$, $\text{C}_3\text{-7-oxacycloalkyl}$; $\text{R}2 = \text{alkyl}$, aryl , alkyl-aryl , $\text{CH}_2\text{-aryl}$, $\text{CHar}_2\text{-aryl}$, vinyl , alkynyl , propynyl , allyl , 3,3-dialkylallyl , E or 2-haloalkenyl , 3,3-dihaloallyl , $\text{C}_3\text{-7-cycloalkyl}$, $\text{CHar}_2\text{-n}$, $\text{C}_3\text{-7-oxacycloalkyl}$, alkylpropynyl , $\text{C}_3\text{-7-alkylallyl}$, 3,3-dialkylallyl , A (joined at X); B1 , B2 = single or E^- , Z^- , B/Z -double bond; B1 = epoxide; $\text{B4} = \text{H, F, Cl, Br, I, alkyl}$ (esp. $\text{Me, Et, propynyl, allyl, 3,3-dialkylallyl, C}_3\text{-7-cycloalkyl}$, $\text{CHar}_3\text{-n}$, $\text{C}_3\text{-7-oxacycloalkyl}$, $\text{E} = \text{Me, CH}_2\text{OH, CH}_2\text{-PG, CHO, CO}_2\text{PG, CH}_2\text{-halo, CONH}_2\text{PG, CONHMe, CN; R} = \text{alkyl, Nu} = \text{R4 O-PG OR, N(PG)}_2$, N(alkyl)_2 , S-PG , S-alkyl Se-PG , Se-alkyl CN , N3 , aryl, heteroaryl ; $\text{PG} = \text{protective group}$), their derivs., a method for the prodrn. thereof and the use of the same for producing epothilones B and D and their derivs. esp. relates to the prodrn. of acyloins in a non-racemic form by means of diastereomer sepn. or synthesis using auxiliary agents and by means of enzymic resoln. of racemates. The invention also relates to epothilone synthesis components, a method for the prodrn. thereof and the use of synthesis components for producing epothilones and

REFERENCE COUNT: 31

THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15. ANSWER 9 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:314889 CAPLUS
16:340534
TITLE: Method for the production of asymmetrically substituted acyloins and derivatives and for the production of epothilones B and D and their derivatives
INVENTOR(S): Uwe Henke, Lukas A.; Scheid, Guenther; Bornscheuer, Morphchem A.-G., Germany
PATENT ASSIGNEE(S): PCT Int. Appl., 182 pp.
SOURCE: CODEN: PIXD2

their derivs. Thus, optically active (Z)-3-hydroxy-6,10-dimethyl-11-[(tert-butyldimethylsilyl)oxy]undeca-5,9-dien-2-one via enzymic resoln. with Chiazyme L6. The optically active hydroxy ketone was converted to three 3-O-(tert-butyldimethylsilyl)epothilone D stereoisomers. 104621-48-9

IT

RL: Cat. (Catalyst use); USES (Uses)

(propn. of asym. substituted acyloins and derivs. for the of epothilone B, D and their derivs.)

RN

9001-62-1, lipase 104439-77-2

CN

Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 9016-88-6, CAPLUS

CN Ruthenium bis(acetato- kappa.O., kappa.O')[(1R)-[1,1'-binaphthalene]-2,2'-diyl]bis(diphenylphosphine- kappa.P)]-, (OC-6-22-.DBLTA.)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104621-48-9, CAPLUS

CN Ruthenium bis(acetato- kappa.O., kappa.O')[(1R)-[1,1'-binaphthalene]-2,2'-diyl]bis(diphenylphosphine- kappa.P)]-, (OC-6-22-.DBLTA.)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 9001-62-1, CAPLUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2, CAPLUS

CN Ruthenium tetracarbonyl-mu-hydro[[1,2,3,4,5-,eta.,-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

PAGE 1-A

(Me2CH)2N], undergoes hydrolysis with lithium hydroxide in methanol followed by acidic lactonization to give the nonracemic γ -lactone II in 92% ee.

IT 9001-62-1, lipase 104439-77-2

RL: Cat. (Catalyst use); USES (Uses) (enantioselective prep. of γ -hydroxy acid derivs. by either kinetic or dynamic kinetic resoln. of γ -hydroxy acid derivs. with Pseudomonas cepacia lipase in absence or presence of Ruthenium rhenium catalyst)

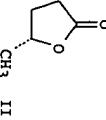
CN 9001-62-1, CAPLUS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2, CAPLUS

CN Ruthenium tetracarbonyl-mu-hydro[[1,2,3,4,5-,eta.,-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

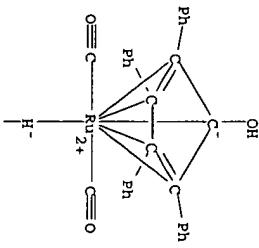
PAGE 1-A



AB .gamma.-Hydroxy acid derivs. MeCH(OR)CH2CH2COR1 [R = H; R1 = Me3CO,

(Me2CH)2N] (I) undergo enzymic kinetic resoln. with 4-chlorophenyl acetate in the presence of *Pseudomonas cepacia* lipase to give nonracemic I (R = Ac) in 44-56% yields and in 77-99% ee.

When the enzymic resoln. is performed under anaerobic conditions in the presence of a bis(hydroxycyclopentadienyl)diruthenium tetracarbonyl hydride resoln. catalyst and in the presence of 2,4-dimethyl-3-pentanol as a hydride donor, nonracemic I (R = Ac) is isolated in 43-93% yields and in 71-98% ee from the dynamic kinetic resoln. MeCH(OC(=O)CH2CH2CON(CMe2)2, prep. in 93% yield and 98% ee from the dynamic kinetic resoln. of I [R = H; R1 =



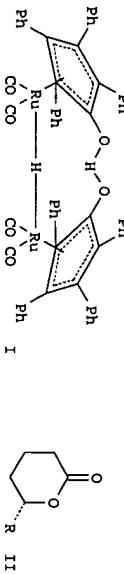
PAGE 2-A

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESION NUMBER: 2002:64783 CAPLUS
 DOCUMENT NUMBER: 136:263059
 TITLE: Enzymatic kinetic resolution and
 chemoenzymatic dynamic kinetic resolution of chiral
 .delta.-hydroxy esters. An efficient route to chiral
 .delta.-lactones
 Pamies, Oscar; Brækvall, Jan-E.
 Arrhenius Laboratory, Department of Organic Chemistry,
 Stockholm University, Stockholm, SE-106 91, Swed.
 Journal of Organic Chemistry (2002), 67(4), 1261-1265
 CODEN: JOCEAH ISSN: 0022-2633
 AMERICAN Chemical Society
 Journal
 English
 CASREACT 136:263059

AUTHOR(S):
 CORPORATE SOURCE:
 SOURCE:
 PUBLISHER:
 DOCUMENT TYPE:
 LANGUAGE:
 OTHER SOURCE(S):
 GI



III

AB Racemic .delta.-hydroxy esters $\text{RCH}(\text{OH})\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}_2\text{CMe}_3$ ($\text{R} = \text{Me}$, Et) underwent kinetic **resolin**, by lipase-catalyzed transesterification with 4-chlorophenyl acetate in toluene to give nonracemic .delta.-acetoxyl acetoxyl acetate ($\text{R} = \text{Me}$, Et) and the (S)-.delta.-hydroxy esters $\text{RCH}(\text{OH})\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}_2\text{CMe}_3$ ($\text{R} = \text{Et}$) in 98-99% ee (E value up to 360). When the Sharpless ruthenium isomerization catalyst I was added to the enzymatic acylation conditions, the combination of the enzymatic kinetic **resolin**, with a ruthenium-catalyzed alc. **racemization** led to an efficient dynamic kinetic **resolin**, of the .delta.-hydroxy esters to give (R)- $\text{RCH}(\text{OAc})\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}_2\text{CMe}_3$ in 87-89% yields and in ee up to 99%. The .delta.-hydroxy esters were converted to .delta.-lactones II, important building blocks in the synthesis of natural products and biol. active compds., by deacetylation with lithium hydroxide in toluene/methanol followed by acidification with hydrochloric acid. (S)-5-(tert-butylidimethylsilyl)-heptanal ($\text{S}-\text{EtCH}(\text{OBn})\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO}$ (TBMS = tert-butylidimethylsilyl)), a key intermediate in the synthesis of widely used com. insecticide Spinosyn A, was prep'd from (S)-EtCH(OH)CH₂CH₂CH₂CO₂CMe₃ by silylation of the secondary alc. followed by reacn. of the ester with disobutylaluminum hydride. 9001-62-1, Lipase

IT: CAPLUS (Catalyst use); USES (Uses)

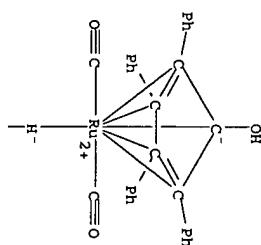
(Pseudomonas cepacia); enantioselective prepn. of .delta.-lactones by dynamic kinetic **resolin**, of .delta.-hydroxy esters by acylation with 4-chlorophenyl acetate in presence of Lipase and ruthenium isomerization catalyst

RN: 9001-62-1 CAPLUS
 Lipase, triacylglycerol (SG1) (CA INDEX NAME)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 IT: 10439-77-2
 RU: CAPLUS (Catalyst use); USES (Uses)
 (enantioselective prepn. of .delta.-lactones by dynamic kinetic

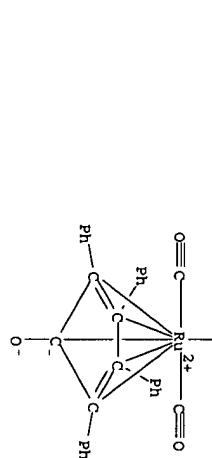
resolin, of .delta.-hydroxy esters by acylation with 4-chlorophenyl acetate in presence of lipase and ruthenium isomerization catalyst)

RN: 104439-77-2 CAPLUS
 CN: Ruthenium, tetracarbonyl-mu-hydro((1,2,3,4,5-.eta.)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl)di- (gci) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESION NUMBER: 2001:868714 CAPLUS
 DOCUMENT NUMBER: 136:770
 TITLE: Process for the preparation of enantiomerically enriched esters and alcohols
 INVENTOR(S): Gerardus, Gerhardus Karel Marin; De Vries, Johannes Verzijl; Gerardus, Broxterman, Quirinus Bernardus DSM N.V., Neth.

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 43 pp.

PAGE 1-A

DOCID: PIXX02

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2001090396 A1 20011129 WO 2001-01383 20010521

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KB, KR, KZ, LC, LK, LR,

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, TT,

RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, UA, UG, US, UZ,

VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, ZH, AT, BE,

CH, CY, ES, SI, SZ, TZ, UC, ZG, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,

JP 2003153993 T2 20031118 JP 2001-586591 20010521

PRIO. APPLN. INFO.: NL 2000-1015313 A 20000526

NL 2000-0101313 NL 2000-00526 NO 2001-01333 W 20010521

EP 1203898 A1 20030219 EP 2001-032416 20010521

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

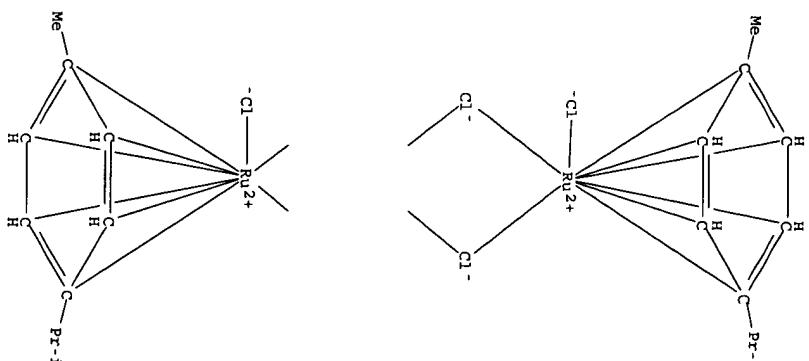
IE, SI, IT, LV, FI, RO, MK, AL, TR

OTHER SOURCE(S): CASREACT 136:4770; MARPAT 136:4770

AB Method for the prepn. of an enantiomerically enriched ester, in which a mixt. of the enantiomers of the correspondingly enriched secondary alc. is subjected in the presence of an acyl donor, to an enantioselective conversion in the presence of a racemization catalyst upon which the ester is formed and an acyl donor residue is obtained, and in which the acyl donor residue is irreversibly removed from the phase in which the enantioselective conversion takes place. Preferably the enantioselective conversion is carried out enzymatically and a transfer hydrogenation catalyst is used as racemization catalyst. The secondary alc. can be formed in situ from the corresponding ketone, in the presence of a H donor. It is also possible to use a mixt. of the secondary alc. and the corresponding ketone as substrate. Preferably the acyl donor is chosen so that the acyl donor residue is converted in situ into another compd. and/or the acyl donor residue is removed via distn. under reduced pressure. The enantiomerically enriched esters obtained can subsequently be converted into the corresponding enantiomerically enriched alcs., which are desirable intermediate products in the prepn. of liq. crystals, agro chems. or pharmaceuticals.

IT RU:CAT (Catalyst use); USSS (Uses)
(prepns. of enantiomerically enriched esters and alcs.)RN 9001-02-1 Capnus
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 52462-29-0 Capnus
CN Ruthenium, di-*mu*-chlorodichlorobis([1,2,3,4,5,6-eta]-1-methyl-4-(1-methylethyl)benzene)di- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 104429-77-2 CAPNUS
CN Ruthenium, tetracarbonyl-*mu*-hydro[1,2,3,4,5-eta]-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

PAGE 1-A

AB An efficient kinetic **resoln.** of **racemic** **beta**-**hydroxy** nitriles was performed via *Candida antarctica* lipase (N-435) -catalyzed transesterification. A variety of **racemic** aryl-aryl, and aryloxymethyl substituted **beta**-**hydroxy** nitriles was efficiently transformed to the corresponding enantiomerically pure acetates (ee >99%) and conversion = 50% with E values from 40 to >1000. The combination of the enzymic kinetic **resoln.** with a ruthenium-catalyzed alc. **racemization** led to a dynamic kinetic **resoln.** (ee's up to 99%, yields up to 65%).

IT 9001-62-1, Lipase 10439-77-2

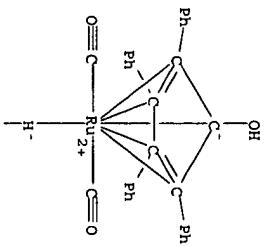
RU: CAT (Catalyst use); USES (Uses)

(1-lipase-catalyzed kinetic **resoln.** and dynamic kinetic **resoln.** of **beta**-**hydroxy** nitriles)

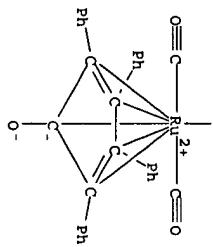
RN 9001-62-1, CAPUS, Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

4 RN 104439-77-2, CAPLUS
CN Ruthenium, tetracarbonyl-*mu*-**hydro**[(1,2,3,4,5-*eta*)-1-**hydroxy**lato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-*yl*]*di*- (9CI) (CA INDEX NAME)



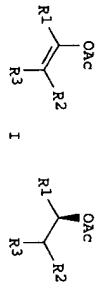
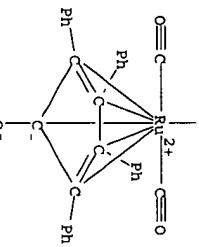
PAGE 1-A



PAGE 2-A

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE IN THE RE FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001-669911 CAPLUS
DOCUMENT NUMBER: 136:37080
TITLE: Efficient lipase-catalyzed kinetic **resolution** and dynamic kinetic **resolution** of **beta**-**hydroxy** nitriles: A route to useful precursors for **beta**-**gamma**-**amino** alcohols
AUTHOR(S): Pamela Oscar, Backvall, Jan-E. CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, 106 91, Swed.
SOURCE: Advanced Synthesis & Catalysis (2001), 34(6+7), 726-731
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2004 ACS ON STN
ACCESSION NUMBER: 2001:416874 CAPLUS

TITLE: 133:19231

INVENTOR(S): Stereoselective method for preparing chiral esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution. Park, Jai Wook; Kim, Jeong Hwan; Jung, Byun Min

PATENT ASSIGNEE(S): Samsung Fine Chemicals Co., Ltd.; S. Korea; Pohang University of Science and Technology

SOURCE: PCT Int. Appl., 19 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

PATENT ACC. NUM. COUNT: 1
PATENT INFORMATION:

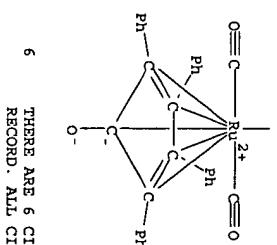
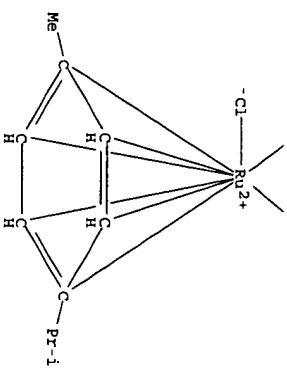
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001040157	A1	20010607	WO 2000-RK1169	20001018
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GR, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, IC, IK, IR, LS, IT, LU, LV, MA, MD, MG, MK, MN, MW, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, RW: GL, GM, NZ, BY, KG, KZ, MD, RU, TJ, TM, TZ, UG, ZW, AT, BB, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SR, BF, BJ, CF, CG, CL, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG	EP 2000-971338	20001018		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, IT, LV, FI, RO, MK, CY, AL	JP 2003519336	20030507	JP 2001-541847	20001018
US 200102898	A1	20010809	US 2000-726412	20001201
US 6475773	B2	20021105	KR 1999-54472	A 19991202
PRIORITY APPLN. INFO.: G1			WO 2000-RK1169	W 20001018
OTHER SOURCE(S): CASREACT 135:19231; MARPAT 135:19231				

AB A method for preg. optically pure chiral esters I (R1, R2 and R3 = independently (un)substituted alkyl, aryl or cycloalkyl group and R1 and R2, R1 and R3, and R2 and R3 can form a cyclic ring; substituent may be halogen or cyano group) in high yield from alkenyl esters via ruthenium catalyzed redn./racemization with successive enzymic reson. is disclosed. For example, II was synthesized in 89% yield (98% enantiomeric excess) by mixing 1-phenylethyl acerate with 2,6-dimethylheptan-4-ol, a ruthenium catalyst, and Novozym 435 followed by heating under Argon with subsequent chromatog. purifn. The chiral esters obtained can be used as synthetic intermediates for preg. various chiral compds. chiral pharmaceutical drugs (e.g. Atorvastatin and Agenetase) or chiral agrochems. (e.g. L-Carnitine). IT 9001:62-1, Novozym 435 52462-29-0 104439-77-2 RU: CAT (catalyst use); USES (Uses)

(stereoselective method for preg. chiral esters from alkenyl esters via ruthenium catalyzed redn. and enzymic reson. of racemic alc. intermediate) IT 9001:62-1, CAPLUS 52462-29-0 CAPLUS CN: Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
CN: Ruthenium, di-mu-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylbutyl)benzene]di-(9CI) (CA INDEX NAME)





REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 15 OF 23 CAPTUS COPYRIGHT 2004 ACS ON STN
ACCESSION NUMBER: 2001-412358 CAPTUS
DOCUMENT NUMBER: 135:152357
TITLE: Lipase/Ruthenium-Catalyzed Dynamic Kinetic Resolution of Hydroxy Acids, Diols, and Hydroxy Aldehydes Protected with a Bulky Group

AUTHOR(S): Hyo-Jin Kim, Main-Joo Choi, Yoon Kyung Choi, Min Young Kim, Mi Jung Park, Jaiwook Rohang, Kyung-Hee Rohang, Kyungbuk, 790-784, S. Korea

CORPORATE SOURCE: National Research Laboratory of Chirotechnology, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, Kyungbuk, 790-784, S. Korea

SOURCE: Journal of Organic Chemistry (2001), 66 (13), 4736-4738
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:152357
AB The racemic title substrates were modified with bulky protecting groups and then subjected to the lipase/ruthenium-catalyzed dynamic kinetic resolution. (DKR). E.g., DCR of $\text{MeCH}(\text{OH})\text{CH}_2\text{CO}_2\text{CH}_2\text{Ph}$ with *Pseudomonas cepacia* lipase, a Ru catalyst, and 4-CloSOAc gave (R)- $\text{MeCH}(\text{OC})\text{CH}_2\text{CO}_2\text{Ph}$ (88% yield, 86 % ee).

IT 9001-62-1, Lipase PSD 104439-77-2

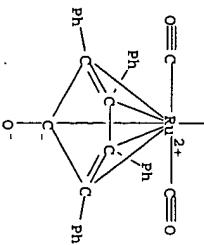
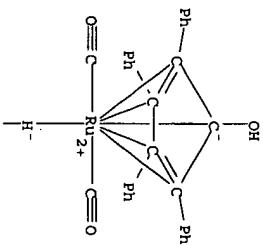
RU: CAT (Catalyst use); USGS (Uses)
(lipase/ruthenium-catalyzed dynamic kinetic resolution of hydroxy acids, diols, and hydroxy aldehydes protected with a bulky group)

RN 9001-62-1 CAPTUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPTUS
CN Ruthenium, tetracarbonyl-mu-hydro[(1,2,3,4,5-eta)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

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REFERENCE COUNT:

15 ANSWER 16 OF 23
CAPLUS COPYRIGHT 2004 ACS ON STN
2001:300657 CAPLUS
134:310984

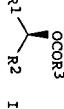
36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 2-A

IT 52462-29-0
RU: CAT (Catalyst use); USES (Uses)

RN 52462-29-0 CAPLUS
CN ruthenium, di- mu -chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-

AB Title esters [1; R1-R3 = (cyclo)alkyl, aryl, etc.] were prep'd. from R1COR2 in the presence of a Ru complex, a lipase, a hydride donor, and an acyl donor wherein unacylated alkanol enantiomer is racemized providing for complete conversion.



PRIORITY APPLN. INFO.: JP 2003512035 T2 20030402
KR 1999-45041 A 19991018
WO 2000-KR1171 W 20001018
OTHER SOURCE(S): CASREACT 134:310984; MARPAT 134:310984
GI

15 ANSWER 16 OF 23
CAPLUS COPYRIGHT 2004 ACS ON STN
2001:300657 CAPLUS
134:310984

TITLE: Preparation of chiral esters

INVENTOR(S): Park, Jai Wook; Kim, Mahn-Joo; Koh, Jeong Hwan; Jung, Hyun Min

PATENT ASSIGNEE(S): Samsung Fine Chemicals Co., Ltd., S. Korea; Pohang University of Science and Technology

SOURCE: PCT Int. Appl., 20 pp.

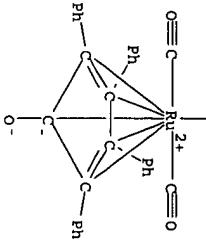
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE



REFERENCE COUNT:

42

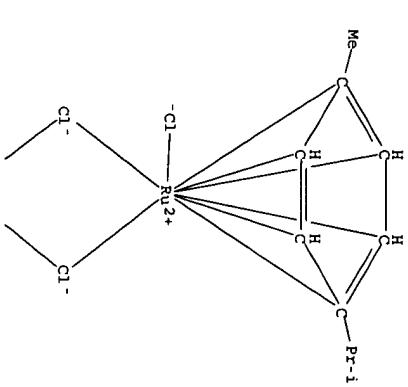
THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2004 ACS ON STN
 ACCESSION NUMBER: 2000:455856 CAPLUS
 DOCUMENT NUMBER: 133122192
 TITLE: Dynamic Kinetic Resolution of Allylic Alcohols Mediated by Ruthenium- and Lipase-Based Catalysts

AUTHOR(S): Lee, Donghyun; Huh, Bun A.; Kim, Mahn-Joo; Jung, Hyun Min; Koh, Jeong Hwan; Park, Jaiwook
 Department of Chemistry, Division of Molecular and Life Science, Pohang University of Science and Technology, Pohang Kyungbuk, 790-784, S. Korea
 SOURCE: Organic Letters, 2(15), 2377-2379
 CODEN: ORCLF7; ISSN: 1523-0060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal

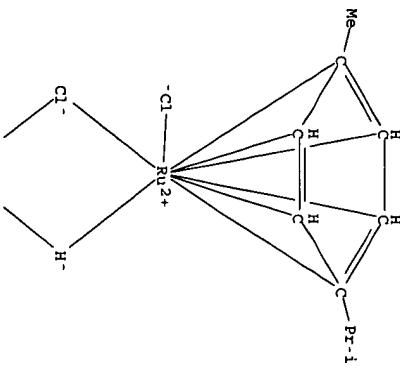
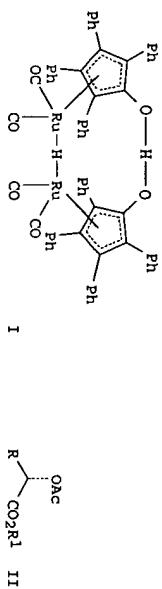
LANGUAGE: English
 OTHER SOURCE(S): CA/REACT 133:122192
 AB An enzyme-metal combo reaction has been developed for the dynamic kinetic resolution of allylic alcs. in which racemic substrates are transformed by a lipase and a ruthenium complex in the presence of an acyl donor to allylic acetates of high optical purity in over 80% yield.
 IT 9001-62-1, Lipase
 RU: C4T (catalyst use); USSS (Uses)
 (catalyst for enantioselective acylation of racemic allylic alcs.; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic alcs. and Ru-catalyzed racamization of unreacted substrate)

RN 9001-62-1, CAPLUS
 CN Lipase, triacylglycerol (9C1) (CA INDEX NAME)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 IT 52462-29-0, (p-Cymene)ruthenium(II) chloride dimer
 90720-60-8, Ruthenium, -mu,-chlorodichloro,-mu,-hydrobis[(1,2,3,4,5,6,-eta.)-1-methyl-1-(1-methylethyl)benzene] di- (racemization catalyst for dynamic kinetic resoln of allylic alcs.; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic alcs. and Ru-catalyzed racamization of unreacted substrate)
 RN 52462-29-0, CAPLUS
 Ruthenium, di,-mu,-chlorodichlorobis[(1,2,3,4,5,6,-eta.)-1-methyl-1-(1-methylethyl)benzene]di- (9C1) (CA INDEX NAME)



RN 90720-60-8 CAPLUS
 CN Ruthenium, -mu,-chlorodichloro,-mu,-hydrobis[(1,2,3,4,5,6,-eta.)-1-methyl-4-(1-methylethyl)benzene] di- (racemization catalyst for dynamic kinetic resoln of allylic alcs.; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic alcs. and Ru-catalyzed racamization of unreacted substrate)

PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE (S): CASREACT 132:333983
 GI



AB Enzymic **resoln.** of α -hydroxy esters $\text{RCH}(\text{OH})\text{CO}_2\text{R}_1$ ($\text{R} = \text{Bu}^\circ$, Ph , $4\text{-MeOC}_6\text{H}_4$, PhCH_2CH_2 , $4\text{-BrC}_6\text{H}_4$, cyclohexyl; $\text{R}_1 = \text{Me}$, Et) in combination with ruthenium-catalyzed **racemization** with the dimeric ruthenium catalyst I led to dynamic **resoln.** of the α -hydroxy esters to give esters II in good yields and excellent 'ee's'. E.g., Me - α -hydroxy- 4 -methoxyphenylacetate and 4 -chlorophenylacetate were dissolved in cyclohexane; argon was bubbled through the soin, and the soin was injected by cannula into a Schlenk flask with 2 mol% catalyst I and 30 mg of *Pseudomonas cepacia* lipase and heated for 48 h and 60°C . to give acetate III ($\text{R} = 4\text{-MeOC}_6\text{H}_4$; $\text{R}_1 = \text{Me}$) in 76% yield and in 94% ee.

IT 9001-62-1, Lipase 52462-29-0

RU: CNT (Catalyst use); USES (Uses)

(nonracemic prepn. of α -hydroxy esters by dynamic **resoln.**

. in the presence of *Pseudomonas cepacia* lipase and a diruthenium catalyst)

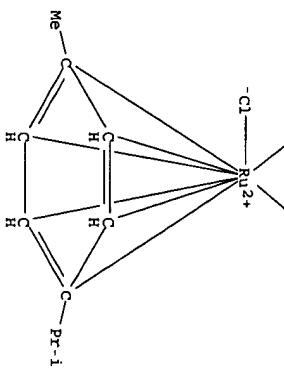
RN 9001-62-1, CAPIUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 52462-29-0, CAPIUS

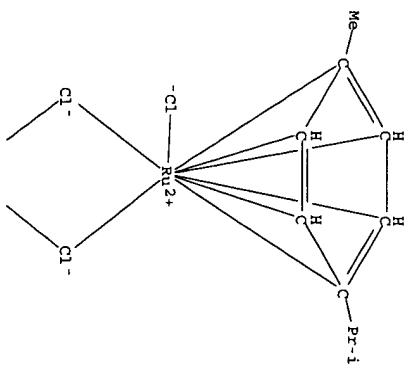
CN Ruthenium, di- μ -chlorodichlorobis[(1,2,3,4,5,6- eta)-1-methyl-4-(1-methylethyl)benzene]di- (9CI) (CA INDEX NAME)



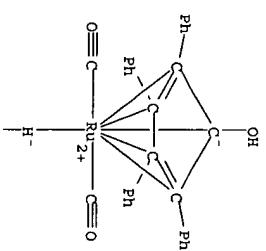
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

US ANSWER 19 OF 23 CAPLUS COPYRIGHT 2004 ACS ON STN
 ACCESSION NUMBER: 2000:1:96518 CAPLUS
 DOCUMENT NUMBER: 132:333983
 TITLE: Dynamic Kinetic Resolution of
 α -hydroxy Acid Esters
 AUTHOR(S): Huerta, Fernando F.; Laxmi, Y. R. Santosh; Baeckvall,
 Jan-E. Department of Organic Chemistry Arrhenius laboratory,
 Stockholm University, Stockholm, SE-106 91, Swed.
 CORPORATE SOURCE: Organic Letters (2000), 2(8), 1037-1040
 SOURCE: CODEN: ORLEF7; ISSN: 1523-7060

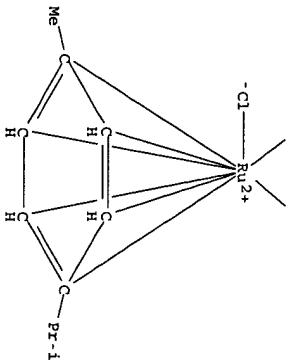
PAGE 1-A



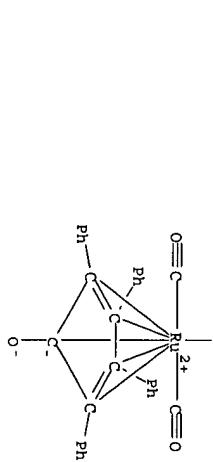
PAGE 1-A



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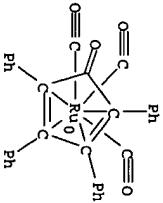
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IT 104439-77-2P
RL: CAY (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
. In the presence of Pseudomonas cepacia lipase and a diruthenium (nonracemic prep. of alpha-hydroxy esters by dynamic **zeolin** catalyst)
RN 104439-77-2 CAYUS
2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl)[(1,2,3,4,5-eta)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

RN CN



REFERENCE COUNT:

17

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESION NUMBER: 1999:379055 CAPLUS
 DOCUMENT NUMBER: 131:123567
 TITLE: Dynamic Kinetic Resolution of Secondary
 Diols via Coupled Ruthenium and Enzyme Catalysis

AUTHOR(S): Persson, B.; Anders; Huerta, Fernando F.; Baeckvall, Jan-E.
 CORPORATE SOURCE: Department of Organic Chemistry, Uppsala University, Uppsala, SE-751 21, Swed.
 SOURCE: Journal of Organic Chemistry (1999), 64(14), 5237-5240
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal

LANGUAGE: English

CASBATT 131:129567

AB Enzymic acylation of secondary sym. diols (as meso/dL mixts.) in combination with ruthenium-catalyzed isomerization of the diol led to efficient dynamic kinetic resoln. In this way, a meso/dL mixt. of the diol was transformed to enantioselectively pure (R,R)-diacetate, making efficient use of all the diol material. For some of the flexible substrates, substantial amts. of meso-diacetates were formed as side products. The results indicate that the major part of the meso product is formed via an intramol. acyl-transfer pathway.

IT 9001-62-1, Novorm 435 104435-77-2
 RL: CAT (catalytic use); USES (USES)

(dynamic kinetic resoln. of secondary diols via coupled

ruthenium and enzyme catalysis)

RN 9001-62-1 CAPLUS
 CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

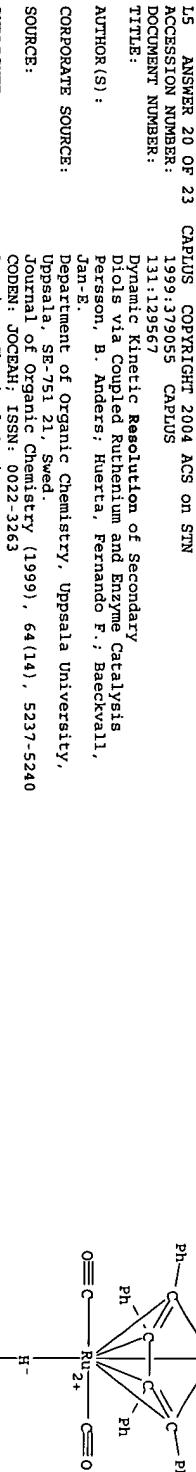
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104435-77-2 CAPLUS
 CN Ruthenium, tetracarbonyl-mu-hydro[[1,2,3,4,5-etc.]-1-hydroxy-ato-2,3,4,5-tetraphenyl-2,4-cyclpentadien-1-yl]di- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

29

THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



15 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESION NUMBER: 1998:332954 CAPLUS
 DOCUMENT NUMBER: 129:95085
 TITLE: Asymmetric Diels-Alder reaction via enzymic kinetic

resoln. using enchyvinyl methyl fumarate Kita, Yasuyuki; Imanishi, Masashi; Akai, Shuji; Matsugi, Masato
 CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, Osaka University, Osaka, 565, Japan
 SOURCE: Chemical Communications (Cambridge) (1998), (11), 1183-1184
 CODEN: CICCP5; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A domino-type asym. [4+2] cycloaddn. reaction following TOYOBO LIP

enzymic kinetic resoln. using ethoxyvinyl Me fumarate is

IT 9001-62-1, Lipase 52462-29-0

KU: C4I (catalyst use); USES (uses) (aSv/m²): Diels-Alder reaction via enzymic kinetic resolution: using

ethoxyvinyl Me fumarate)

9001-62-1 CARLOS
[j,passe, triacylglycerol] (act) (CA INDEX NAME)

STRUCTURE DIAGRAM IS NOT AVAILABLE ***
52463-29-0 CAPIVIS

Ruthenium, di-*mu*-chlorodichlorobis[(1,2,3,4,5,6--eta)-1-methyl

methyl ethyl benzene]di- (9CI) (CA INDEX NAME)

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15 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1998-16459 CAPLUS
 DOCUMENT NUMBER: 128-23199
 TITLE: Synthesis of 4-Sulfur-Substituted (2S,3R)-3-
 Phenylsirines by Enzymic Resolution.
 Enantiopure Precursors for Thiamphenicol and
 Flufenicol
 AUTHOR(S): Kaptein, Bernard; van Dooren, Thei J. G. M.; Boesten,
 Wilhelms H. J.; Sonke, Theo; Duchateau, Alexander L.
 L.; Broekerman, Quirinus B.; Kamhuis, Johan
 CORPORATE SOURCE: Organic Chemistry Biotechnology Section, Fine
 Chemicals, DSM Research, Geleen, 6160 MD, Neth.
 SOURCE: Organic Process Research & Development (1998), 2(1),
 10-17
 CODEN: OPRDKP; ISSN: 1083-6160
 REFERENCE COUNT: 17
 THERE ARE 17 CITED REFERENCES AVAILABLE IN THE REFORMAT

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREF 128:23109
67



AB
enantiomerically pure 4-methylthio- and 4-methylsulfonyl-substituted

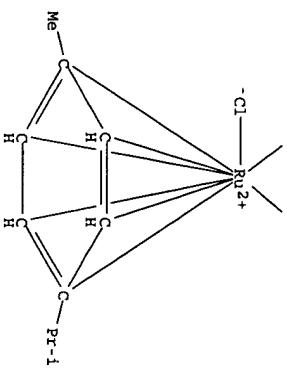
racemic α -, β -, γ -, δ -phenylserines I ($R = Mes$, $MesO2$) are prepd. by enzymatic reduction of the corresponding **racemic** threo amides using the amidease from *Ochrobactrum anthropi* NCIMB 40221. The unwanted (2R,3S)-amide enantiomers are sepd. from the enantiopure amino acids and easily racemized after Schiff base formation with the corresponding 4-(methylthio)- and 4-(methylsulfonyl)benzaldehyde. The racemization can be combined with the prepn. of the **racemic** amides by alcohol reaction under crystn. conditions to yield only the three isomers. Enantiopure phenylserines I ($R = Mes$, $MesO2$) are thus obtained in 78% and 62% overall yields starting from the corresponding substituted benzaldehydes. I ($R = Mes$) is reduced to diol II with $NaBH_4$ /H₂SO₄ and can be used for the synthesis of thiamphenicol and florfenicol.

II with NaBH₄/H₂SO₄ and can be

IT
9001-62-1, Lipase 109361-17-3
RL: CAT (Catalyst use); USES (Uses
Lipase use).

**(asym. synthesis of sulfur-substituted phenylserines by enzymic
reduc. of racemic anides and racemisation
of unwanted stereoisomers.)**

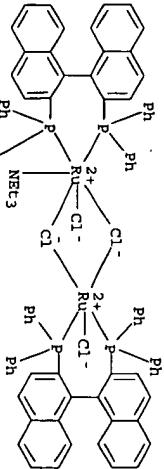
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CN

Ruthenium, tetracarbonyl-mu-hydro[1,2,3,4,5-eta.]-1-hydroxylato-
2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (SCI) (CA INDEX NAME)

PAGE 1-A



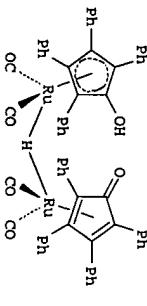
REFERENCE COUNT:

15 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2004 ACS ON STN
1997:407237 CAPLUS
127:135610

TITLE: Enzymic resolution of alcohols coupled with
ruthenium-catalyzed racemization of the
substrate alcohol
Larsson, Anna L. E.; Persson, B. Anders; Backvall,
Jan-E.
Department Organic Chemistry, Uppsala University,
Uppsala, S-75121, swed.

Source: Angewandte Chemie, International Edition in English
(1997), 36(11), 1211-1212
CODEN: ACIEAY; ISSN: 0570-0833
Wiley-VCH
Journal
English
CASREACT 127:135610

DOCUMENT TYPE:
PUBLISHER:
LANGUAGE:
OTHER SOURCE(S):
G1
C



AB

The ruthenium-catalyzed **racemization** of (+)-(R)-.alpha.-
methylbenzenemethanol was coupled with an enzyme-catalyzed
transesterification to give the resolved alc. deriv. Thus, the
combination of catalyst I, 4-chlorophenyl acetate and Novozym 435 in the
reaction of (+)-(R)-.alpha.-methylbenzenemethanol gave
(R)-.alpha.-methylbenzenemethanol acetate in high yield and high
enantiomeric purity.

IT 9001-22-1, Novozym 435 104439-77-2
RL: CAP (catalyst used); USBS (Used)
(ruthenium-catalyzed **racemization** and sequential enzymic
resoln. of alcs.)

RN 9001-22-1, CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 104439-77-2 CAPLUS

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